

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:sssptal626gms

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

\* \* \* \* \* Welcome to STN International \* \* \* \* \*

NEWS 1 Web Page URLs for STN Seminar Schedule - N. America  
NEWS 2 Apr 08 "Ask CAS" for self-help around the clock  
NEWS 3 Apr 09 BEILSTEIN: Reload and Implementation of a New Subject Area  
NEWS 4 Apr 09 ZDB will be removed from STN  
NEWS 5 Apr 19 US Patent Applications available in IFICDB, IFIPAT, and IFIUDB  
NEWS 6 Apr 22 Records from IP.com available in CAPLUS, HCAPLUS, and ZCAPLUS  
NEWS 7 Apr 22 BIOSIS Gene Names now available in TOXCENTER  
NEWS 8 Apr 22 Federal Research in Progress (FEDRIP) now available  
NEWS 9 Jun 03 New e-mail delivery for search results now available  
NEWS 10 Jun 10 MEDLINE Reload  
NEWS 11 Jun 10 PCTFULL has been reloaded  
NEWS 12 Jul 02 FOREGE no longer contains STANDARDS file segment  
NEWS 13 Jul 22 USAN to be reloaded July 28, 2002;  
saved answer sets no longer valid  
NEWS 14 Jul 29 Enhanced polymer searching in REGISTRY  
NEWS 15 Jul 30 NETFIRST to be removed from STN  
NEWS 16 Aug 08 CANCERLIT reload  
NEWS 17 Aug 08 PHARMAMarketLetter(PHARMAML) - new on STN  
NEWS 18 Aug 08 NTIS has been reloaded and enhanced  
NEWS 19 Aug 19 Aquatic Toxicity Information Retrieval (AQUIRE)  
now available on STN  
NEWS 20 Aug 19 IFIPAT, IFICDB, and IFIUDB have been reloaded  
NEWS 21 Aug 19 The MEDLINE file segment of TOXCENTER has been reloaded  
NEWS 22 Aug 26 Sequence searching in REGISTRY enhanced  
NEWS 23 Sep 03 JAPIO has been reloaded and enhanced  
NEWS 24 Sep 16 Experimental properties added to the REGISTRY file  
NEWS 25 Sep 16 Indexing added to some pre-1967 records in CA/CAPLUS  
NEWS 26 Sep 16 CA Section Thesaurus available in CAPLUS and CA  
  
NEWS EXPRESS February 1 CURRENT WINDOWS VERSION IS V6.0d,  
CURRENT MACINTOSH VERSION IS V6.0a(ENG) AND V6.0Ja(JP),  
AND CURRENT DISCOVER FILE IS DATED 05 FEBRUARY 2002  
NEWS HOURS STN Operating Hours Plus Help Desk Availability  
NEWS INTER General Internet Information  
NEWS LOGIN Welcome Banner and News Items  
NEWS PHONE Direct Dial and Telecommunication Network Access to STN  
NEWS WWW CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

All use of STN is subject to the provisions of the STN Customer agreement. Please note that this agreement limits use to scientific research. Use for software development or design or implementation of commercial gateways or other similar uses is prohibited and may

result in loss of user privileges and other penalties.

\* \* \* \* \* STN Columbus \* \* \* \* \*

FILE 'HOME' ENTERED AT 16:18:41 ON 22 SEP 2002

=> FIL REGISTRY  
COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
0.21	0.21

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 16:18:53 ON 22 SEP 2002  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
COPYRIGHT (C) 2002 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file  
provided by InfoChem.

STRUCTURE FILE UPDATES: 20 SEP 2002 HIGHEST RN 453593-49-2  
DICTIONARY FILE UPDATES: 20 SEP 2002 HIGHEST RN 453593 49 2

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

Please note that search-term pricing does apply when  
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

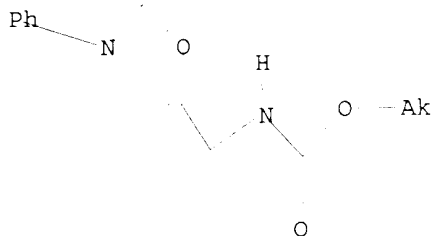
Experimental and calculated property data are now available. See HELP  
PROPERTIES for more information. See STNote 27, Searching Properties  
in the CAS Registry File, for complete details:  
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=>  
Uploading 09982157.str

L1 STRUCTURE UPLOADED

=> d l1  
L1 HAS NO ANSWERS  
L1 STR

O



Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 16:19:17 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 31 TO ITERATE

100.0% PROCESSED 31 ITERATIONS  
SEARCH TIME: 00.00.01

0 ANSWERS

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 286 TO 954  
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s l1 sss full

FULL SEARCH INITIATED 16:19:23 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 745 TO ITERATE

100.0% PROCESSED 745 ITERATIONS  
SEARCH TIME: 00.00.01

1 ANSWERS

L3 1 SEA SSS FUL L1

=> FIL CAPLUS  
COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
140.28	140.49

FULL ESTIMATED COST

FILE 'CAPLUS' ENTERED AT 16:19:35 ON 22 SEP 2002  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
COPYRIGHT (C) 2002 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 22 Sep 2002 VOL 137 ISS 13  
FILE LAST UPDATED: 20 Sep 2002 (20020920/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

CAS roles have been modified effective December 16, 2001. Please check your SDI profiles to see if they need to be revised. For information on CAS roles, enter HELP ROLES at an arrow prompt or use the CAS Roles thesaurus (/RL field) in this file.

=> d his

Golam Shameem

(FILE 'HOME' ENTERED AT 16:18:41 ON 22 SEP 2002)

FILE 'REGISTRY' ENTERED AT 16:18:53 ON 22 SEP 2002

L1 STRUCTURE UPLOADED

L2 0 S L1

L3 1 S L1 SSS FULL

FILE 'CAPLUS' ENTERED AT 16:19:35 ON 22 SEP 2002

=> s l3

L4 2 L3

=> d ibib abs hitstr l4 tot

L4 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1989:8198 CAPLUS

DOCUMENT NUMBER: 110:8198

TITLE: Preparation of (aminomethyl)phenyloxazolidinones as antibacterial agents

INVENTOR(S): Gregory, Walter A.

PATENT ASSIGNEE(S): du Pont de Nemours, E. I., and Co., USA

SOURCE: U.S., 47 pp. Cont.-in-part of U.S. Ser. No. 676,745, abandoned.

CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

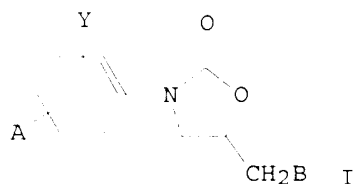
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4705799	A	19871110	US 1985-803191	19851202
CA 1254213	A1	19890516	CA 1984-455844	19840605
ZA 8404265	A	19860129	ZA 1984-4265	19840606
HU 196771	B	19890130	HU 1987-5132	19840606
IL 77230	A1	19900610	IL 1985-77230	19851204
CA 1275652	A2	19901030	CA 1988-580778	19881020
NO 8902178	A	19841210	NO 1989-2178	19890530
NO 169122	B	19920203		
NO 169122	C	19920513		

PRIORITY APPLN. INFO.:

US 1983-501897	19830607
US 1984-578332	19840214
US 1984-676745	19841205
CA 1984-455844	19840605
IL 1984-72028	19840605
NO 1984-2273	19840606
CA 1985-455844	19850402

OTHER SOURCE(S): CASREACT 110:8198

GI



AB The title compds. [I; A = NO<sub>2</sub>, SH, alkylsulfonyl, -sulfinyl, -sulfenyl, etc.; B = N<sub>3</sub>, (substituted) amino; Y = H, F, Cl, Br, alkyl, NO<sub>2</sub>; or AY = O(CH<sub>2</sub>)<sub>n</sub> where n = 1, 2, or 3], useful as antibacterial agents for mammals, are prepd. A mixt. of I (A = 4-MeSO<sub>2</sub>, B = OSO<sub>2</sub>C<sub>6</sub>H<sub>4</sub>Me-4, Y = H) (prepn. given) and NaN<sub>3</sub> in DMF was heated at 90-100.degree. for 1 h to give I (A = 4-MeSO<sub>2</sub>, B = N<sub>3</sub>, Y = H). = H) (II). II showed a minimal inhibition concn. of 6.3 .mu.g/mL against Staphylococcus epidermidis.

IT **96800-18-9**

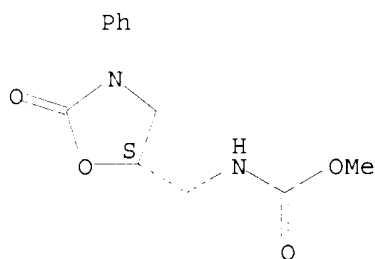
RL: RCT (Reactant)

(reaction of, in prepn. of antibacterial phenyloxazolidinones)

RN 96800-18-9 CAPLUS

CN Carbamic acid, [(2-oxo-3-phenyl-5-oxazolidinyl)methyl]-, methyl ester, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1985:437470 CAPLUS

DOCUMENT NUMBER: 103:37470

TITLE: Aminomethyloxooxazolidinylbenzene derivatives useful as antibacterial agents

INVENTOR(S): Gregory, Walter Adelman

PATENT ASSIGNEE(S): du Pont de Nemours, E. I., and Co. , USA

SOURCE: Eur. Pat. Appl., 85 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

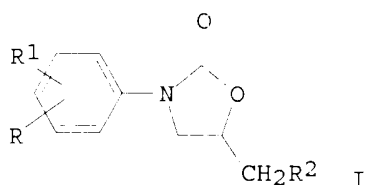
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 127902	A2	19841212	EP 1984-106400	19840605
EP 127902	A3	19870902		
EP 127902	B1	19911016		
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
ES 533097	A1	19850801	ES 1984-533097	19840604
AU 8429099	A1	19841213	AU 1984-29099	19840605
AU 583250	B2	19890427		
IL 72028	A1	19880531	IL 1984-72028	19840605
CA 1254213	A1	19890516	CA 1984-455844	19840605
AT 68490	E	19911115	AT 1984-106400	19840605
FI 8402273	A	19841208	FI 1984-2273	19840606
FI 83216	B	19910228		
FI 83216	C	19910610		
DK 8402795	A	19841208	DK 1984-2795	19840606
NO 8402273	A	19841210	NO 1984-2273	19840606

NO 163451	B	19900219		
NO 163451	C	19900530		
JP 60008277	A2	19850117	JP 1984-114710	19840606
HU 34462	A2	19850328	HU 1984-2192	19840606
HJ 194194	B	19880128		
ZA 8404265	A	19860129	ZA 1984-4265	19840606
HU 196771	B	19890130	HU 1987-5132	19840606
SU 1505442	A3	19890830	SU 1984-3752502	19840606
ES 540812	A1	19880316	ES 1985-540812	19850228
SU 1426451	A3	19880923	SU 1986-4024095	19860207
CA 1275652	A2	19901030	CA 1988-580778	19881020
NO 8902178	A	19841210	NO 1989-2178	19890530
NO 169122	B	19920203		
NO 169122	C	19920513		

PRIORITY APPLN. INFO.:

US 1983-501897	19830607
US 1984-578332	19840214
CA 1984-455844	19840605
EP 1984-106400	19840605
NO 1984-2273	19840606
CA 1985-455844	19850402

GI



AB The bactericidal oxazolidinones I [R = e.g. NO<sub>2</sub>, cyano, HO, HS, (un)substituted amines, alkylsulfonyl, alkylthio, alkylsulfinyl, aryl, sulfamoyl, alkoxy, or carbamoyl; R<sub>1</sub> = H, F, Cl, Br, NO<sub>2</sub>; RR<sub>1</sub> = alkylenedioxy, R<sub>2</sub> = NH<sub>2</sub>, acylamino, N<sub>3</sub>, alkylsulfonylamino, alkylsulfinylamino] and their physiol. acceptable salts were prepd. Thus, (.-.-)-I (R = 4-MeSO<sub>2</sub>, R<sub>1</sub> = H, R<sub>2</sub> = Cl) was treated with NaI and the resulting (.-.-)-I (R<sub>2</sub> = iodo) treated with NaN<sub>3</sub> followed by hydrogenation in F<sub>3</sub>CCO<sub>2</sub>H to give (.-.-)-I (R = 4-MeSO<sub>2</sub>; R<sub>1</sub> = H, R<sub>2</sub> = NH<sub>2</sub>).F<sub>3</sub>CCO<sub>2</sub>H (II). The min. inhibitory concn. of II was 50 .mu.g/mL against Staphylococcus epidermidis.

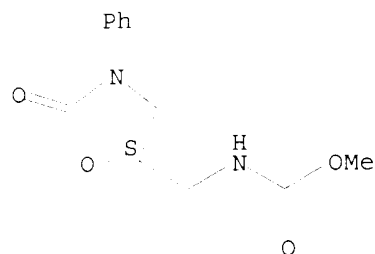
IT **96800-18-9P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)  
(prepn. and chlorosulfonylation of)

RN 96800-18-9 CAPLUS

CN Carbamic acid, [(2-oxo-3-phenyl-5-oxazolidinyl)methyl]-, methyl ester,  
(S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



=> FIL REGISTRY  
COST IN U.S. DOLLARS

SINCE FILE ENTRY	TOTAL SESSION
9.57	150.06

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE ENTRY	TOTAL SESSION
-1.24	-1.24

CA SUBSCRIBER PRICE

FILE 'REGISTRY' ENTERED AT 16:20:43 ON 22 SEP 2002  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
COPYRIGHT (C) 2002 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 20 SEP 2002 HIGHEST RN 453593-49-2  
DICTIONARY FILE UPDATES: 20 SEP 2002 HIGHEST RN 453593-49-2

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:  
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=>

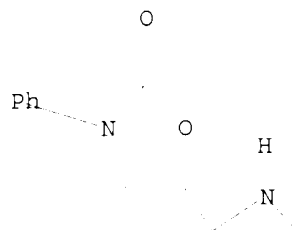
Uploading 09982157a.str

L5 STRUCTURE UPLOADED

=> d 15

L5 HAS NO ANSWERS

L5 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 15

SAMPLE SEARCH INITIATED 16:21:06 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 274 TO ITERATE

100.0% PROCESSED 274 ITERATIONS  
SEARCH TIME: 00.00.01

1 ANSWERS

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 4487 TO 6473  
PROJECTED ANSWERS: 1 TO 80

L6 1 SEA SSS SAM L5

=> s 15 sss full

FULL SEARCH INITIATED 16:21:14 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 6097 TO ITERATE

100.0% PROCESSED 6097 ITERATIONS  
SEARCH TIME: 00.00.01

14 ANSWERS

L7 14 SEA SSS FUL L5

=> FIL CAPLUS

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
140.28	290.34

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
0.00	-1.24

CA SUBSCRIBER PRICE

FILE 'CAPLUS' ENTERED AT 16:21:20 ON 22 SEP 2002  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
COPYRIGHT (C) 2002 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing



of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 22 Sep 2002 VOL 137 ISS 13  
FILE LAST UPDATED: 20 Sep 2002 (20020920/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

CAS roles have been modified effective December 16, 2001. Please check your SDI profiles to see if they need to be revised. For information on CAS roles, enter HELP ROLES at an arrow prompt or use the CAS Roles thesaurus (/RL field) in this file.

=> d his

(FILE 'HOME' ENTERED AT 16:18:41 ON 22 SEP 2002)

FILE 'REGISTRY' ENTERED AT 16:18:53 ON 22 SEP 2002

L1 STRUCTURE UPLOADED  
L2 0 S L1  
L3 1 S L1 SSS FULL

FILE 'CAPLUS' ENTERED AT 16:19:35 ON 22 SEP 2002

L4 2 S L3

FILE 'REGISTRY' ENTERED AT 16:20:43 ON 22 SEP 2002

L5 STRUCTURE UPLOADED  
L6 1 S L5  
L7 14 S L5 SSS FULL

FILE 'CAPLUS' ENTERED AT 16:21:20 ON 22 SEP 2002

=> s 17

L8 19 L7

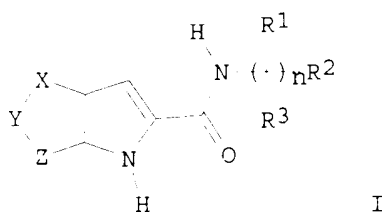
=> d ibib abs hitstr 18 tot

L8 ANSWER 1 OF 19 CAPLUS COPYRIGHT 2002 ACS  
ACCESSION NUMBER: 2002:185126 CAPLUS  
DOCUMENT NUMBER: 136:247485  
TITLE: Preparation of bicyclic pyrrolyl amides as glycogen phosphorylase inhibitors  
INVENTOR(S): Bartlett, Julie B.; Freeman, Sue; Kenny, Peter; Morley, Andrew; Whittamore, Paul  
PATENT ASSIGNEE(S): Astrazeneca AB, Swed.  
SOURCE: PCT Int. Appl., 141 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

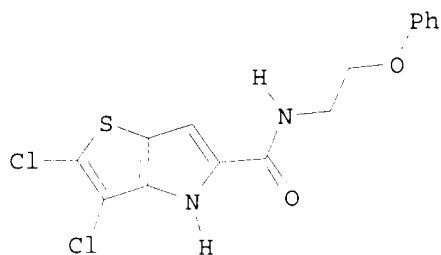
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002020530	A1	20020314	WO 2001-SE1880	20010831
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL,				

PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG,  
 US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM  
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,  
 DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,  
 BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

AU 2001082833 A5 20020322 AU 2001-82833 20010831  
 PRIORITY APPLN. INFO.: GB 2000-21831 A 20000906  
 WO 2001-SE1880 W 20010831  
 OTHER SOURCE(S): MARPAT 136:247485  
 GI



I



II

AB Title compds. I [R1 = H, halo, NO2, CN, OH, (un)substituted alkyl, alkenyl, etc.; R2 = H, halo, NO2, CH2F, CHF2, CF3, amino, alkyl, alkenyl, alkoxy, etc.; R3 = H, alkyl; -X-Y-Z- is selected from -S-CR4=CR5-, -CR4=CR5-S-, -O-CR4=CR5-, -CR4=CR5-O-, -N=CR4-S-, -S-CR4=N-, -NR3-CR4=CR5- and -CR4=CR5-NR3- wherein R4 and R5 = independently H, halo, CN, alkyl, ureido, NO2, etc.; n = 0-4] or a pharmaceutically acceptable salt or an in vivo hydrolyzable ester thereof were prepd. possessing glycogen phosphorylase inhibitory activity (no data). Thus, II was prepd. by amidation of 5-carboxy-2,3-dichloro-4H-thieno[3,2-b]pyrrole with 2-phenoxyethylamine. As glycogen phosphorylase inhibitors, I have value in the treatment of disease states assocd. with increased glycogen phosphorylase activity, e.g., type 2 diabetes. Pharmaceutical compns. contg. I are described.

# IT 403859-17-6P

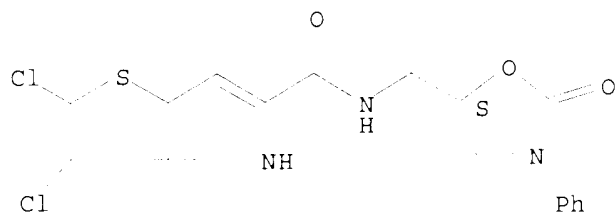
FL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(target compd.; prepn. of thienopyrrolyl amides as glycogen phosphorylase inhibitors)

RN 403859-17-6 CAPLUS

CN 4H-Thieno[3,2-b]pyrrole-5-carboxamide, 2,3-dichloro-N-[[[(5S)-2-oxo-3-phenyl-5-oxazolidinyl]methyl]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 2 OF 19 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2001:827024 CAPLUS

DOCUMENT NUMBER: 136:177462

TITLE: Three-dimensional quantitative structure-activity relationship (3D-QSAR) of 3-aryloxazolidin-2-one antibacterials

AUTHOR(S): Karki, Rajeshri G.; Kulkarni, Vithal M.

CORPORATE SOURCE: Department of Chemical Technology, Pharmaceutical Division, University of Mumbai, Mumbai, Matunga, 400019, India

SOURCE: Bioorganic & Medicinal Chemistry (2001), 9(12), 3153-3160

CODEN: BMECEP; ISSN: 0968-0896

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Three-dimensional quant. structure-activity relation (3D-QSAR) studies for 3-aryloxazolidin-2-one antibacterials were performed using the genetic function approxn. algorithm. This study was performed using 60 compds., in which the QSAR models were developed using a training set of 50 compds. The in vitro min. inhibitory concn. (MIC) against Staphylococcus aureus SFCO-1a was used for the study. The predictive ability of the QSAR model was evaluated by using a test set of 10 compds. The statistical quality of the QSAR models was assessed using statistical parameters  $r^2$ ,  $r^2_{cv}$  (cross-validated  $r^2$ ),  $r^2_{pred}$  (predictive  $r^2$ ) and lack of fit measure (LOF). The results obtained indicate that the antibacterial activity of the 3-aryloxazolidin-2-ones is strongly dependent on electronic factor as expressed by LUMO energy (LUMO), spatial factor as expressed by d. and thermodyn. factors accounted for by molar refractivity and heat of formation. The model is presently being used to design and predict new potent mols. prior to synthesis.

IT 96800-17-8

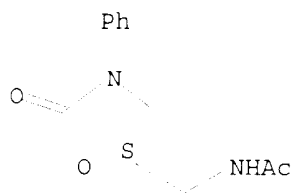
RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(3D-QSAR of antibacterial 3-aryloxazolidin-2-one)

RN 96800-17-8 CAPLUS

CN Acetamide, N-[[[(5S)-2-oxo-3-phenyl-5-oxazolidinyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 3 OF 19 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2001:580914 CAPLUS

DOCUMENT NUMBER: 135:318442

TITLE: Synthesis of oxazolidinones by a solid-phase/activation cycloelimination (SP/ACE) methodology  
AUTHOR(S): ten Holte, Peter; Van Esseveldt, Bart C. J.; Thijs, Lambertus; Zwanenburg, Binne

CORPORATE SOURCE: Department of Organic Chemistry, NSR Institute for Molecular Structure, Design and Synthesis, University of Nijmegen, Nijmegen, 6525 ED, Neth.

SOURCE: European Journal of Organic Chemistry (2001), (15), 2965-2969

CODEN: EJOCFK; ISSN: 1434-193X

PUBLISHER: Wiley-VCH Verlag GmbH

DOCUMENT TYPE: Journal

LANGUAGE: English

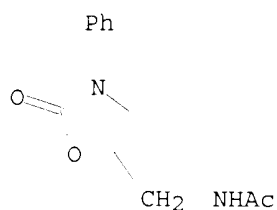
AB A versatile method for the solid-phase synthesis of 3,5-disubstituted oxazolidin-2-ones is described. An appropriate 1,2-diol is attached to immobilized sulfonyl chloride, resulting in the selective activation of one of the alc. functions. The subsequent reaction of the other alc. group with an isocyanate, followed by a base-promoted cycloelimination, gives an oxazolidinone. By proper choice of isocyanates, functionalities can be introduced which are essential for antibiotic activity.

IT 367925-77-7P 367925-78-8P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of oxazolidinones from 1,2-diols and isocyanates by solid phase/activation cycloelimination)

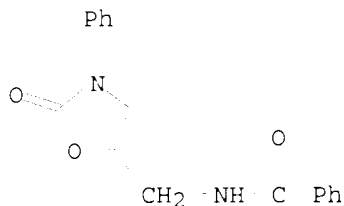
RN 367925-77-7 CAPLUS

CN Acetamide, N-[(2-oxo-3-phenyl-5-oxazolidinyl)methyl]- (9CI) (CA INDEX NAME)



RN 367925-78-8 CAPLUS

CN Benzamide, N-[(2-oxo-3-phenyl-5-oxazolidinyl)methyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 4 OF 19 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2001:392067 CAPLUS

DOCUMENT NUMBER: 135:5606

TITLE: Preparation of oxazolidinones as bactericides

INVENTOR(S): Gordeev, Mikhail F.; Luehr, Gary W.; Patel, Dinesh V.; Ni, Zhi-jie; Gordon, Eric

PATENT ASSIGNEE(S): Pharmacia & Upjohn Company, USA

SOURCE: U.S., 104 pp., Cont.-in-part of U.S. Ser. No. 12,535, abandoned.

CODEN: USXXAM

DOCUMENT TYPE: Patent

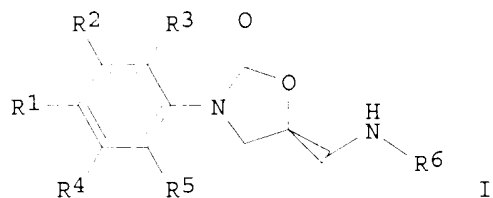
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6239152	B1	20010529	US 1999-235771	19990122
PRIORITY APPLN. INFO.:			US 1998-12535	B2 19980123
			US 1998-86702	B2 19980528

OTHER SOURCE(S): MARPAT 135:5606  
GI



AB Title compds. [e.g., I; R = H; R1 = SR11, CONR7R8, etc.; R7,R8,R11 = H, alkyl, (hetero)aryl, etc.] were prepd. Thus, 3,4-F(Me3CO2C)C6H3NHCO2CH2Ph (prepn. given) was cyclocondensed with (R)-glycidyl butyrate and the product converted in several steps to I (R = resin, R1 = CO2C6F5) which was amidated by morpholine to give, after resin cleavage, I (R = H, R1 = CONHR8, R8 = morpholino). Data for biol. activity of I were given.

IT 96800-17-8P

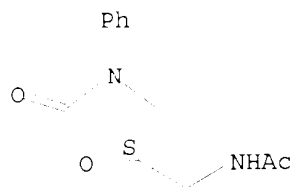
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of oxazolidinones as bactericides)

RN 96800-17-8 CAPLUS

CN Acetamide, N-[[[(5S)-2-oxo-3-phenyl-5-oxazolidinyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 157 THERE ARE 157 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 5 OF 19 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1999:747431 CAPLUS

DOCUMENT NUMBER: 131:351320

TITLE: Preparation of oxazolidinylmethyldithiocarbamic acid derivatives as bactericides and fungicides

INVENTOR(S): Yoshida, Toshihiko; Tokuyama, Tatsuteru; Tomita, Yayoi

PATENT ASSIGNEE(S): Hokurika Pharmaceutical Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 90 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

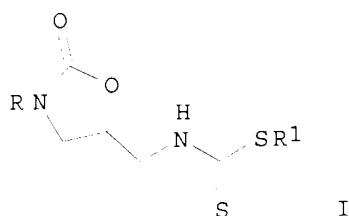
LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 11322729	A2	19991124	JP 1999-57378	19990304
PRIORITY APPLN. INFO.:			JP 1998-74982	19980309
OTHER SOURCE(S):		MARPAT 131:351320		

GI



AB Title compds. I (R = Ph, substituted Ph; R1 = alkyl, cycloalkyl, aryl, aralkyl, etc.) and their salts, useful as bactericides and fungicides, are prepd. Thus, reaction of (S)-5-aminomethyl-2-oxo-3-[4-(thiomorpholin-4-yl)phenyl]oxazolidine with CS<sub>2</sub> in CH<sub>2</sub>Cl<sub>2</sub> in the presence of Et<sub>3</sub>N gave, after treatment with MeI, Me (S)-N-[2-oxo-3-[4-(thiomorpholin-4-yl)phenyl]oxazolidin-5-yl]methyldithiocarbamate. Me (S)-N-[2-oxo-3-[3-fluoro-4-(thiomorpholin-4-yl)phenyl]oxazolidin-5-yl]methyldithiocarbamate showed bactericidal activity superior to that of linezolid.

IT 250373-87-6P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);

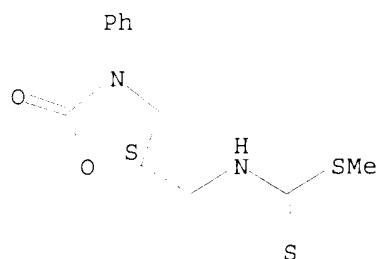
Golam Shameem

BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (prepn. of oxazolidinylmethyldithiocarbamic acid derivs. as  
 bactericides and fungicides)

RN 250373-87-6 CAPLUS

CN Carbamodithioic acid, [[(5S)-2-oxo-3-phenyl-5-oxazolidinyl]methyl]-,  
 methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L8 ANSWER 6 OF 19 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1999:487281 CAPLUS

DOCUMENT NUMBER: 131:116228

TITLE: Preparation of oxazolidinones as bactericides

INVENTOR(S): Gordeev, Mikhail F.; Luehr, Gary W.; Patel, Dinesh V.;  
 Ni, Zhi-Jie; Gordon, Eric

PATENT ASSIGNEE(S): Versicor, Inc., USA

SOURCE: PCT Int. Appl., 229 pp.

CODEN: PIXXD2

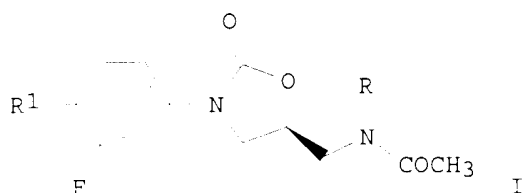
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9937630	A1	19990729	WO 1999-US1318	19990122
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2318969	AA	19990729	CA 1999-2318969	19990122
AU 9924644	A1	19990809	AU 1999-24644	19990122
EP 1049682	A1	20001108	EP 1999-904193	19990122
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2002501059	T2	20020115	JP 2000-528553	19990122
PRIORITY APPLN. INFO.:				
			US 1998-12535	A 19980123
			US 1998-86702	A 19980528
			WO 1999-US1318	W 19990122
OTHER SOURCE(S): MARPAT 131:116228				
GI				



AB Title compds. [e.g., I; R = H; R1 -SR11, CONR7R8, etc.; R7,R8. R11 = H, alkyl, (hetero)aryl, etc.] were prepd. Thus, 3,4-F(Me3CO2C)C6H3NHCO2CH2Ph (prepn. given) was cyclocondensed with (R)-glycidyl butyrate and the product converted in several steps to I (R = resin, R1 = CO2C6F5) which was amidated by morpholine to give, after resin cleavage, I (R = H, R1 = CONHR8, R8 = morpholino). Data for biol. activity of I were given.

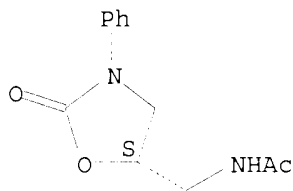
IT 96800-17-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(prepn. of oxazolidinones as bactericides)

RN 96800-17-8 CAPLUS

CN Acetamide, N-[[[(5S)-2-oxo-3-phenyl-5-oxazolidinyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 7 OF 19 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1999:429192 CAPLUS

DOCUMENT NUMBER: 131:184892

TITLE: A short synthesis of oxazolidinone derivatives  
Linezolid and Eperezolid: a new class of  
antibacterials

AUTHOR(S): Lohray, Braj B.; Baskaran, Sundarababu; Rao, B.  
Srinivasa; Reddy, B. Yadi; Rao, I. Nageswara

CORPORATE SOURCE: Basic Research & Drug Discovery, Dr. Reddy's Research  
Foundation, Hyderabad, 500 050, India

SOURCE: Tetrahedron Letters (1999), 40(26), 4855-4856  
CODEN: TELEAY; ISSN: 0040-4039

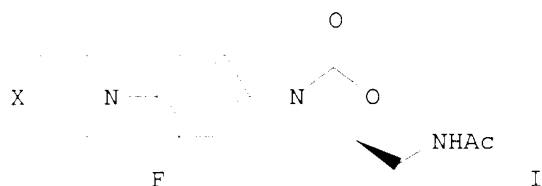
PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

GI





AB Oxazolidinone derivs. such as Linezolid (I, X = O) and Eperezolid (I, X = HOCH<sub>2</sub>CON) have been synthesized from 1,2,5,6-dianhydro-3,4-isopropylidene-D-mannitol in good yield.

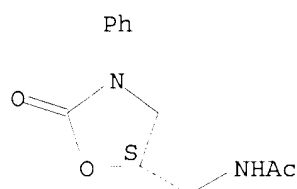
IT **96800-17-8P**

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of oxazolidinone antibacterials)

RN 96800-17-8 CAPLUS

CN Acetamide, N-[[[(5S)-2-oxo-3-phenyl-5-oxazolidinyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 8 OF 19 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1999:194131 CAPLUS

DOCUMENT NUMBER: 130:223265

TITLE: Preparation of N-(2-oxothiazolidin-5-ylmethyl)thiourea derivatives as antibacterial agents

INVENTOR(S): Yoshida, Toshihiko; Tokuyama, Ryukou; Tomita, Yayoi

PATENT ASSIGNEE(S): Hokuriku Seiyaku Co., Ltd., Japan

SOURCE: PCT Int. Appl., 137 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

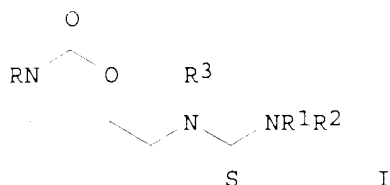
LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9912914	A1	19990318	WO 1998-JP4074	19980910
W:	AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IS, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			

JP 11158164 A2 19990615 JP 1998-272500 19980909  
 AU 9890015 A1 19990329 AU 1998-90015 19980910  
 PRIORITY APPLN. INFO.: JP 1997-265054 19970911  
 WO 1998-JP4074 19980910  
 OTHER SOURCE(S): MARPAT 130:223265  
 GI



AB Antimicrobial thiourea derivs. of general formula (I) or salts thereof: (wherein R1, R2, and R3 are each hydrogen, alkyl, cycloalkyl, nitrogen-protecting group, alkoxycarbonylalkyl or the like; and R is Ph which may be substituted by halogeno, hydroxyl, mercapto, amino, cyano, nitro, carboxyl, carbamoyl, alkyl, cycloalkyl, alkoxy, alkylamino, alkanoyl, arylcarbonyl, aryl, aralkyl, aryloxy, cycloalkyloxy contg. a hetero-atom as a ring atom, a satd. heterocyclic group or the like) are prepd. Also claim is an antibacterial agent, in particular against gram pos. bacteria, contg. I as the active ingredient. These thiourea derivs. exhibit excellent antibacterial activity against not only normal bacteria but also resistant strains of bacteria, e.g. methicillin-resistant *Staphylococcus aureus* (MRSA). Thus, addn. reaction of (R)-[2-oxo-3-[4-(thiomorpholin-4-yl)phenyl]oxazolidin-5-yl]methyl isothiocyanate with NH<sub>3</sub> in MeOH at room temp. for 9 h gave I [R = 4-(thiomorpholin-4-yl)phenyl, R1 = R2 = R3 = H]. I [R = 3-fluoro-4-(pyrrolidino-1-yl)phenyl, R1 = R2 = R3 = H] showed min. inhibitory concn. of 0.39 .mu.g/mL against MRSA HPC1336 and *Enterococcus faecalis* HPC948 and HPC975.

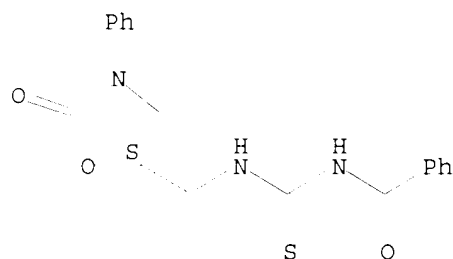
IT 221202-57-9P 221202-58-0P 221202-76-2P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (prepn. of N-(oxothiazolidinylmethyl)thiourea derivs. as antibacterial agents)

RN 221202-57-9 CAPLUS

CN Benzamide, N-[[[(5S)-2-oxo-3-phenyl-5-oxazolidinyl]methyl]amino]thioxomethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

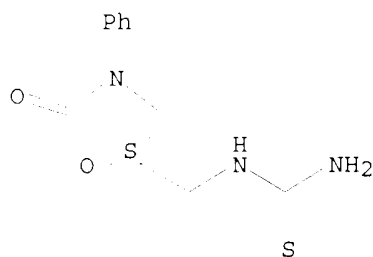


RN 221202-58-0 CAPLUS

Golam Shameem

CN Thiourea, [[(5S)-2-oxo-3-phenyl-5-oxazolidinyl]methyl]- (9CI) (CA INDEX NAME)

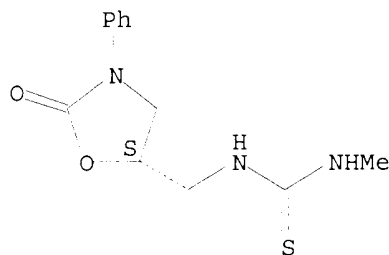
Absolute stereochemistry. Rotation (-).



RN 221202-76-2 CAPLUS

CN Thiourea, N-methyl-N'-[[5S)-2-oxo-3-phenyl-5-oxazolidinyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 9 OF 19 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1992:151623 CAPLUS

DOCUMENT NUMBER: 116:151623

TITLE: Antibacterials. Synthesis and structure-activity studies of 3-aryl-2-oxooxazolidines. 4. Multiply-substituted aryl derivatives

AUTHOR(S): Park, Chung Ho; Brittelli, David R.; Wang, C. L. J.; Marsh, Frank D.; Gregory, Walter A.; Wuonola, Mark A.; McRipley, Ronald J.; Eberly, Virginia S.; Slee, Andrew M.; Forbes, Martin

CORPORATE SOURCE: Drug Discovery Res., Chem. Sci., Exp. Stn., Du Pont Merck Pharm. Co., Wilmington, DE, 19880-0353, USA

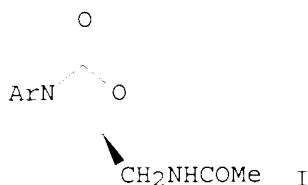
SOURCE: J. Med. Chem. (1992), 35(6), 1156-65

CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



AB The synthesis and structure-activity relationship (SAR) studies of the effect of different polysubstitution patterns in the arom. ring of 5-(acetamidomethyl)oxazolidinones, e.g., (I Ar = substituted Ph, 5-indolyl, .beta.-naphthyl) on antibacterial activity are presented. Compds. I were prepd. by the six-step synthesis described previously via electrophilic arom. substitution reactions of 3-substituted compds., and functional-group interchange reactions of 3,4-disubstituted compds. Antibacterial evaluation of compds. I against *Staphylococcus aureus* and *Enterococcus faecalis* gave the following results. The 2,4- and 2,5-disubstituted derivs. have weak or no antibacterial activity. Antibacterial activities of 3,4-disubstituted compds. are comparable to those of the 4-monosubstituted analogs for small 3-substituents (smaller than Br), but decline rapidly for larger 3-substituents. 3,4-Annulated derivs. are comparable in activity to their open-chain analogs. 3,5-Disubstituted and 3,4,5- and 2,4,6-trisubstituted derivs. are devoid of antibacterial activity.

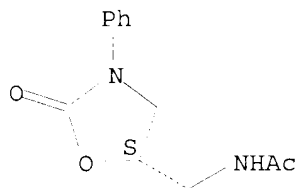
IT 96800-17-8

RL: BAC (Biological activity or effector, except adverse); BIOL  
(Biological study)  
(antibacterial activity of)

RN 96800-17-8 CAPLUS

CN Acetamide, N-[[[(5S)-2-oxo-3-phenyl-5-oxazolidinyl]methyl]- (9CI) (CA  
INDEX NAME)

Absolute stereochemistry.



L8 ANSWER 10 OF 19 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1991:199057 CAPLUS

DOCUMENT NUMBER: 114:199057

TITLE: An automated pulse labelling method for  
structure-activity relationship studies with  
antibacterial oxazolidinones

AUTHOR(S): Eustice, D. C.; Brittelli, D. R.; Feldman, P. A.;  
Brown, L. J.; Borkowski, J. J.; Snee, A. M.

CORPORATE SOURCE: Med. Prod. Dep., E.I. DuPont de Nemours and Co.,  
Wilmington, DE, 19898, USA

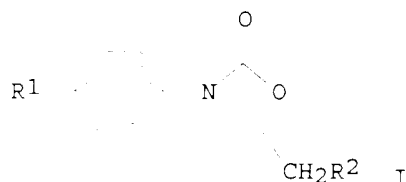
SOURCE: Drugs Exp. Clin. Res. (1990), 16(4), 149-55  
CODEN: DECRDP; ISSN: 0378-6501

DOCUMENT TYPE: Journal

Golam Shameem

LANGUAGE:  
GI

English



AB The 3-aryl-2-oxooxazolidinones (I, R1 = H, SMe, Ac, Me, SMe, SO2Me, NO2, CHMe2, Et; R2 = NHAc, Cl, OH, H, NH2) potentially inhibited protein synthesis. An automated pulse labeling method with [3H]lysine was developed with *Bacillus subtilis* to obtain addnl. quant. activity data for structure-activity relationship studies with the oxazolidinones. Inhibition consts. were calcd. after a Logit fit of the data. When substituents at the 5-Me position of the heterocyclic ring were NHAc, OH, or Cl, the correlation coeff. was 0.87 between the MIC and IC50 (for all compds. with MICs .ltoreq.16 .mu.g/mL). The D-isomers of DuP 721, I (R1 = Ac), and DuP 105, I (R1 = SMe), gave MICs of 128 .mu.g/mL and IC50s of .gtoreq.50 .mu.g/mL for protein synthesis, showing that only the L-isomers were active. By MIC testing, I (R1 = NHAc and R1 = Ac, NO2, SMe, SO2Me, or CHMe2) had comparable antibacterial potency. Pulse labeling anal. showed that I (R1 = Ac or NO2) were more potent inhibitors of protein synthesis.

IT **96800-17-8**

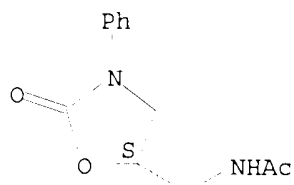
RL: BIOL (Biological study)

(antibacterial activity and structure of, pulse labeling assay for)

RN 96800-17-8 CAPLUS

CN Acetamide, N-[[[(5S)-2-oxo-3-phenyl-5-oxazolidinyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L8 ANSWER 11 OF 19 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1990:532055 CAPLUS

DOCUMENT NUMBER: 113:132055

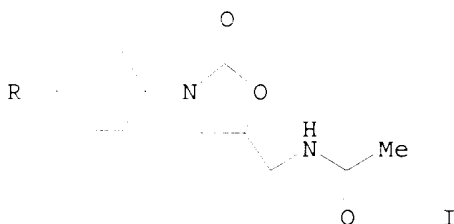
TITLE: Antibacterials. Synthesis and structure-activity studies of 3-aryl-2-oxooxazolidines. 2. The "A" group

AUTHOR(S): Gregory, Walter A.; Brittelli, David R.; Wang, C. L. J.; Kezar, Hollis S., III; Carlson, Randall K.; Park, Chung Ho; Corless, Peter F.; Miller, Steven J.; Rajagopalan, P.; et al.

CORPORATE SOURCE: Med. Prod. Dep., E. I. Du Pont de Nemours and Co., Wilmington, DE, 19880-0353, USA

Golam Shameem

SOURCE: J. Med. Chem. (1990), 33(9), 2569-78  
 CODEN: JMCMAR; ISSN: 0022-2623  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 113:132055  
 GI



AB The synthesis and structure-activity relationship (SAR) studies of the effect of varying the "A" group in a series of 5-(acetamidomethyl)oxazolidinone antibacterials I (R = alkyl, ethenyl, ethynyl, hydroxyalkyl, aldo and keto, oximinoalkyl, carboalkoxy, nitro, amino, halo and .psi.-halo, alkylthio, alkylsulfinyl, alkylsulfonyl) are described. Compds. I were principally prepd. either by the six-step synthesis described previously by elaboration of the synthetic intermediate I (R = H) via electrophilic arom. substitution or elaboration of the intermediate I (R = iodo) by transition metal catalyzed carbon-carbon bond-forming reactions. Antibacterial evaluation of compds. I against Staphylococcus aureus and Enterococcus faecalis led to the identification of several SAR trends. In several series of homolog (alkyl, keto, oximinoalkyl, amino, halo and .psi.-halo, and alkylthio), antibacterial activity increased with increasing lipophilicity. But in series with where R is a substituent with a tri- or tetrasubstituted (substituent larger than H) quaternary atom attached directly to the arom. ring (hydroxyalkyl, alkylsulfinyl, alkylsulfonyl), the activity peaked at the member of the series with the "tert-butyl" connectivity pattern. Conjugated electron-withdrawing substituents also had increased activity relative to nonconjugated analog of comparable lipophilicity.

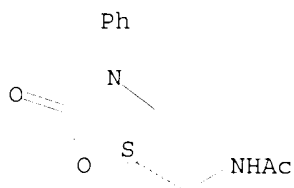
IT 96800-17-8

RL: BAC (Biological activity or effector, except adverse); BIOL (Biological study)  
 (bactericidal activity of)

RN 96800-17-8 CAPLUS

CN Acetamide, N-[[[(5S)-2-oxo-3-phenyl-5-oxazolidinyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

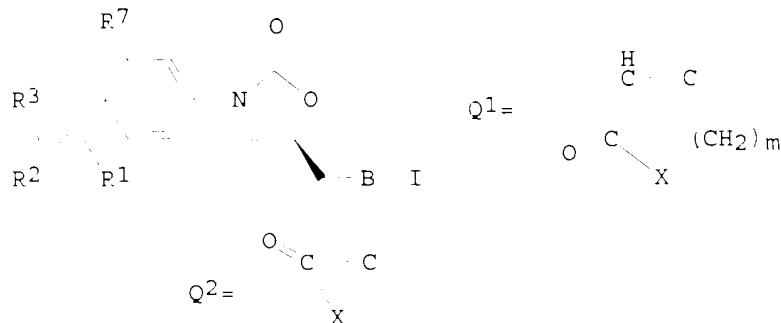


L8 ANSWER 12 OF 19 CAPLUS COPYRIGHT 2002 ACS

Golam Shameem

ACCESSION NUMBER: 1989:632783 CAPLUS  
 DOCUMENT NUMBER: 111:232783  
 TITLE: Preparation and testing of 3-(ethenylphenyl)-5-(aminomethyl)-2-oxooxazolidines as antibacterial agents  
 INVENTOR(S): Brittelli, David Ross; Gregory, Walter Adelman; Corless, Peter Franklin; Park, Chung Ho  
 PATENT ASSIGNEE(S): du Pont de Nemours, E. I., and Co., USA  
 SOURCE: Eur. Pat. Appl., 37 pp.  
 CODEN: EPXXDW  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 316594	A1	19890524	EP 1988-117304	19881018
EP 316594	B1	19930929		
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
CA 1317594	A1	19930511	CA 1988-580498	19881018
AT 95176	E	19931015	AT 1988-117304	19881018
ES 2059467	T3	19941116	ES 1988-117304	19881018
AU 8824043	A1	19890427	AU 1988-24043	19881019
AU 617697	B2	19911205		
DK 8805841	A	19890422	DK 1988-5841	19881020
FI 8804849	A	19890422	FI 1988-4849	19881020
NO 8804676	A	19890424	NO 1988-4676	19881020
JP 01135777	A2	19890529	JP 1988-263043	19881020
ZA 8807853	A	19900627	ZA 1988-7853	19881020
HU 52075	A2	19900628	HU 1988-5417	19881020
HU 201915	B	19910128		
IL 88107	A1	19930221	IL 1988-88107	19881020
SU 1801109	A3	19930307	SU 1988-4356676	19881020
US 4977173	A	19901211	US 1989-376457	19890707
PRIORITY APPLN. INFO.:			US 1987-110837	19871021
			EP 1988-117304	19881018
OTHER SOURCE(S):		MARPAT 111:232783		
GI				



AB The title compds. [I; R1 = H, CF3, (substituted) C1-3 alkyl, Ph; R1R2 = Q1, (CH2)p; R2, R3 = electron withdrawing group, R1; R2R3 = Q2; R4 = H,

C1-10 alkyl, C3-8 cycloalkyl; R5 = H, (substituted) C1-4 alkyl, C2-4 alkenyl, C3-4 cycloalkyl, OR6, CH2OR4; R6 = (substituted) C1-4 alkyl; R7 = H, Me, Et, F, OH; B = NH2, NR4COR5, NR4S(O)uR6, N3; X = CH2, O, S, imino; m = 1-3; n = 2-4; p = 3-5; u = 1,2], useful as antibacterials, were prepd. (EtO)2P(O)CH2CN was added dropwise to NaH in DMF at 5.degree..

L-N-[3-(4-acetylphenyl, 1-2-oxooxazolidin-5-ylmethyl]acetamide was then added and the mixt. was stirred overnight at room temp. to give I (R1 = Me, R2 = CN, R3 = R7 = H, B = NHCOMe). I had min. inhibitory concns. of 0.5->128 .mu.g/mL against Staphylococcus aureus.

IT 96800-17-8

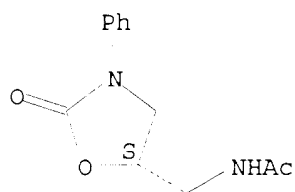
RL: RCT (Reactant)

(reaction of, in prepn. of antibacterial)

RN 96800-17-8 CAPLUS

CN Acetamide, N-[[{(5S)-2-oxo-3-phenyl-5-oxazolidinyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L8 ANSWER 13 OF 19 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1989:574083 CAPLUS

DOCUMENT NUMBER: 111:174083

TITLE: [(Aminomethyl)oxooxazolidinyl]aroylbenzene derivatives useful as antibacterial agents, and their preparation and pharmaceutical compositions

INVENTOR(S): Adelman, Gregory Walter; Smith, Kezar Hollis, III

PATENT ASSIGNEE(S): du Pont de Nemours, E. I., and Co., USA

SOURCE: Eur. Pat. Appl., 19 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 312000	A1	19890419	EP 1988-116903	19881012
EP 312000	B1	19920318		
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
CA 1320730	A1	19930727	CA 1988-579796	19881011
AT 73783	E	19920415	AT 1988-116903	19881012
ES 2033394	T3	19930316	ES 1988-116903	19881012
DK 8805739	A	19890417	DK 1988-5739	19881014
FI 8804755	A	19890417	FI 1988-4755	19881014
NO 8804594	A	19890417	NO 1988-4594	19881014
NO 174551	B	19940214		
JP 01132570	A2	19890525	JP 1988-257417	19881014
HU 49864	A2	19891128	HU 1988-5297	19881014
HU 199810	B	19900328		
ZA 8807683	A	19900627	ZA 1988-7683	19881014
SU 1616517	A3	19901223	SU 1988-4356643	19881014



IL 88047	A1	19921115	IL 1988-88047	19881014
AU 8823962	A1	19890420	AU 1988-23962	19881017
AU 617366	B2	19911128		
US 4942183	A	19900717	US 1989-376456	19890707
PRIORITY APPLN. INFO.:			US 1987-109032	19871016
			EP 1988-116903	19881012

OTHER SOURCE(S): MARPAT 111:174083

GI For diagram(s), see printed CA Issue.

AB Title compds. I [1-isomer or racemic mixt.; R = NH<sub>2</sub>, NR<sub>3</sub>COR<sub>4</sub>, NR<sub>3</sub>S(O)uR<sub>5</sub>, N<sub>3</sub>; R<sub>1</sub> = H and R<sub>2</sub> = H, OH, N(R<sub>6</sub>)<sub>2</sub>; R<sub>1</sub>R<sub>2</sub> = O, NOH, NOR<sub>5</sub>, NOCOR<sub>4</sub>, (4-methylpiperazino)imino; R<sub>3</sub> = H, C<sub>1</sub>-10 alkyl, C<sub>3</sub>-8 cycloalkyl; R<sub>4</sub> = H, C<sub>1</sub>-4 alkyl, C<sub>2</sub>-4 alkenyl, C<sub>3</sub>-4 cycloalkyl, OR<sub>5</sub>; R<sub>5</sub> = C<sub>1</sub>-4 alkyl; R<sub>6</sub> = H, C<sub>1</sub>-4 alkyl; X = Ph or pyridyl (un)substituted by 1-3 of halo, C<sub>1</sub>-4 alkyl, NO<sub>2</sub>, OR<sub>5</sub>, or S(O)mR<sub>5</sub>; m = 0-2] are prep'd. as antibacterials. A mixt. of (MeSO<sub>2</sub>)<sub>2</sub>O, MeSO<sub>3</sub>H, (1)-N-(3-phenyl-2-oxo-5-oxazolidinylmethyl)acetamide, and 4-FC<sub>6</sub>H<sub>4</sub>CO<sub>2</sub>H was stirred at 50-60.degree. to give 73% (1)-I (R = NHAc, R<sub>1</sub>R<sub>2</sub> = O, X = 4-FC<sub>6</sub>H<sub>4</sub>) (II). The ED<sub>50</sub> of II for protection of mice against lethality of i.p. Staphylococcus aureus was 40 mg/kg orally and 20 mg/kg s.c.

IT 96800-17-8

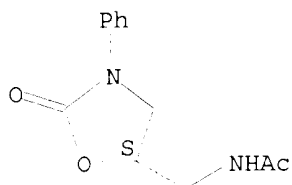
RL: RCT (Reactant)

(reaction of, in prepn. of antibacterial [(aminomethyl)oxooxazolidinyl] aroylbenzene derivs.)

RN 96800-17-8 CAPLUS

CN Acetamide, N-[[[(5S)-2-oxo-3-phenyl-5-oxazolidinyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L8 ANSWER 14 OF 19 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1989:515092 CAPLUS

DOCUMENT NUMBER: 111:115092

TITLE: Chiral synthesis of DuP 721 [(S)-N-[3-(4-acetylphenyl)-2-oxo-5-oxazolidinylmethyl]acetamide], a new antibacterial agent

AUTHOR(S): Wang, Chia Lin J.; Gregory, Walter A.; Wuonola, Mark A.

CORPORATE SOURCE: Med. Prod. Dep., E.I. Du Pont De Nemours Co., Inc., Wilmington, DE, USA

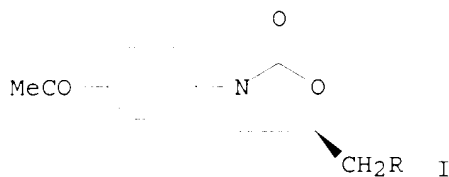
SOURCE: Tetrahedron (1989), 45(5), 1323-6  
CODEN: TETRAB; ISSN: 0040-4020

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 111:115092

GI



AB A 6-step chiral synthesis of the title compd. I (R = NHAc) from 4-MeCOC6H4NCO (II) and (R)-glycidyl butyrate (III) is reported. The reaction of II with III gave I (R = O2CPr), which was hydrolyzed to give I (R = OH). Mesylation of I (R = OH), followed by reaction with NaN<sub>3</sub> gave I (R = N<sub>3</sub>), which as redn. with P(OMe)<sub>3</sub> gave I (R = NH<sub>2</sub>). N-Acetylation of I (R = NH<sub>2</sub>) gave the title compd.

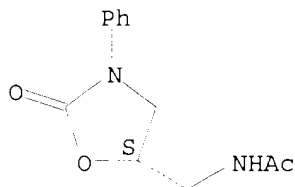
IT **96800-17-8P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. and acetylation of)

RN 96800-17-8 CAPLUS

CN Acetamide, N-[[[(5S)-2-oxo-3-phenyl-5-oxazolidinyl)methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L8 ANSWER 15 OF 19 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1989:457600 CAPLUS

DOCUMENT NUMBER: 111:57600

TITLE: Antibacterials. Synthesis and structure-activity studies of 3-aryl-2-oxooxazolidines. 1. The B group  
AUTHOR(S): Gregory, Walter A.; Brittelli, David R.; Wang, C. L. J.; Wuonola, Mark A.; McRipley, Ronald J.; Eustice, David C.; Eberly, Virginia S.; Snee, Andrew M.; Forbes, Martin; Bartholomew, P. T.

CORPORATE SOURCE: Exp. Stn., E. I. du Pont de Nemours and Co., Wilmington, DE, 19898, USA

SOURCE: J. Med. Chem. (1989), 32(8), 1673-81

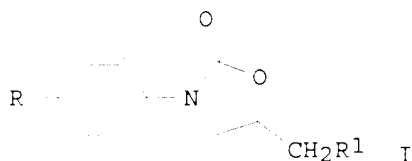
CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 111:57600

GI



AB The synthesis and structure/activity studies of the effect of varying the B group in a series of oxazolidinone antibacterials I (R = Me<sub>2</sub>CH, Me, SO<sub>2</sub>, Ac, etc.; R<sub>1</sub> ident. B = H, Me, OH, NHAc, etc.) are described. Two synthetic routes were used (1) alkylation of aniline with glycidol followed by dialkyl carbonate heterocyclization to afford I (R = H, R<sub>1</sub> .tplbond. B = OH), whose arene ring was further elaborated by using electrophilic arom. substitution methodol.; (2) cycloaddn. of substituted aryl isocyanates with epoxides. I with B = OH or Br were converted to other B functionalities by using SN<sub>2</sub> methodol. Antibacterial evaluation of compds. I with R = acetyl, iso-Pr, methylthio, methylsulfinyl, methylsulfonyl, and sulfonamido and a variety of different .beta. groups against Staphylococcus aureus and Enterococcus faecalis concluded that the compds. with B = aminoacyl, and particularly acetamido, were the most active of those examd. in each R series, possessing MIC's in the range of 0.5-4 .mu.g/mL for the most active compds. described.

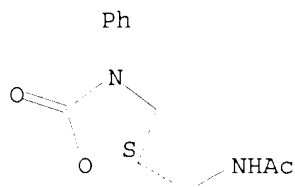
IT **96800-17-8P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)  
(prepn. and reactions of)

RN 96800-17-8 CAPLUS

CN Acetamide, N-[[[(5S)-2-oxo-3-phenyl-5-oxazolidinyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L8 ANSWER 16 OF 19 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1989:8198 CAPLUS

DOCUMENT NUMBER: 110:8198

TITLE: Preparation of (aminomethyl)phenyloxazolidinones as antibacterial agents

INVENTOR(S): Gregory, Walter A.

PATENT ASSIGNEE(S): du Pont de Nemours, E. I., and Co., USA

SOURCE: U.S., 47 pp. Cont.-in-part of U.S. Ser. No. 676,745, abandoned.

CODEN: USXXAM

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

PATENT NO.

KIND DATE

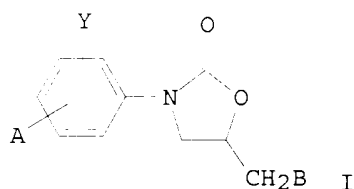
APPLICATION NO. DATE

US 4705799	A	19871110	US 1985-803191	19851202
CA 1254213	A1	19890516	CA 1984-455844	19840505
ZA 8404265	A	19860129	ZA 1984-4265	19840606
HU 196771	B	19890130	HU 1987-5132	19840606
IL 77230	A1	19900610	IL 1985-77230	19851204
CA 1275652	A2	19901030	CA 1988-580778	19881020
NO 8902178	A	19841210	NO 1989-2178	19890530
NO 169122	B	19920203		
NO 169122	C	19920513		

PRIORITY APPLN. INFO.:

US 1983-501897	19830607
US 1984-578332	19840214
US 1984-676745	19841205
CA 1984-455844	19840605
IL 1984-72028	19840605
NO 1984-2273	19840606
CA 1985-455844	19850402

OTHER SOURCE(S): CASREACT 110:8198  
GI



AB The title compds. [I; A = NO<sub>2</sub>, SH, alkylsulfonyl, -sulfinyl, -sulfenyl, etc.; B = N<sub>3</sub>, (substituted) amino; Y = H, F, Cl, Br, alkyl, NO<sub>2</sub>; or AY = O(CH<sub>2</sub>)<sub>n</sub>O where n = 1, 2, or 3], useful as antibacterial agents for mammals, are prepd. A mixt. of I (A = 4-MeSO<sub>2</sub>, B = OSO<sub>2</sub>C<sub>6</sub>H<sub>4</sub>Me-4, Y = H) (prepn. given) and NaN<sub>3</sub> in DMF was heated at 90-100.degree. for 1 h to give I (A = 4-MeSO<sub>2</sub>, B = N<sub>3</sub>, Y = H). = H) (II). II showed a minimal inhibition concn. of 6.3 .mu.g/mL against Staphylococcus epidermidis.

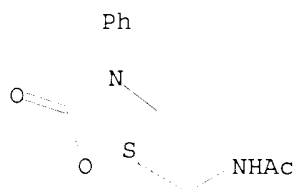
IT **96800-17-8P 96800-36-1P**

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of, as intermediate for antibacterial agents)

RN 96800-17-8 CAPLUS

CN Acetamide, N-[[{(5S)-2-oxo-3-phenyl-5-oxazolidinyl)methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

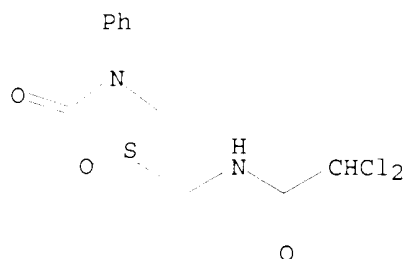


RN 96800-36-1 CAPLUS

CN Acetamide, 2,2-dichloro-N-[(2-oxo-3-phenyl-5-oxazolidinyl)methyl]-, (S)- (9CI) (CA INDEX NAME)

Golam Shameem

Absolute stereochemistry.



IT 96800-17-8 96800-18-9

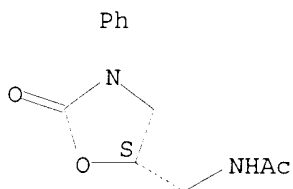
RL: RCT (Reactant)

(reaction of, in prepn. of antibacterial phenyloxazolidinones)

RN 96800-17-8 CAPLUS

CN Acetamide, N-[(5S)-2-oxo-3-phenyl-5-oxazolidinyl]methyl]- (9CI) (CA INDEX NAME)

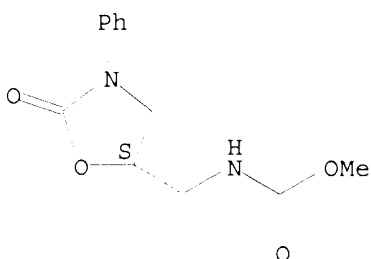
Absolute stereochemistry.



RN 96800-18-9 CAPLUS

CN Carbamic acid, [(2-oxo-3-phenyl-5-oxazolidinyl)methyl]-, methyl ester, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L8 ANSWER 17 OF 19 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1986:572439 CAPLUS

DOCUMENT NUMBER: 105:172439

TITLE: Phenyl(aminomethyl)oxazolidinones as antibacterial agents

INVENTOR(S): Gregory, Walter Adelman

PATENT ASSIGNEE(S): du Pont de Nemours, E. I., and Co., USA

SOURCE: Eur. Pat. Appl., 53 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

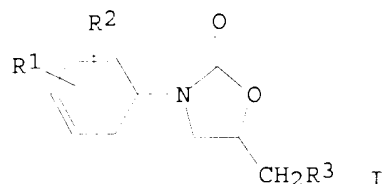
Golam Shameem

FAMILY ACC. NUM. COUNT: 3

## PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 184170	A2	19860611	EP 1985-115243	19851130
EP 184170	A3	19870902		
EP 184170	B1	19911016		
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
CA 1260948	A1	19890926	CA 1985-496421	19851128
AT 68491	E	19911115	AT 1985-115243	19851130
DK 8505618	A	19860606	DK 1985-5618	19851204
DK 169103	B1	19940815		
FI 8504804	A	19860606	FI 1985-4804	19851204
FI 82453	B	19901130		
FI 82453	C	19910311		
NO 8504883	A	19860606	NO 1985-4883	19851204
NO 164540	B	19900709		
NO 164540	C	19901017		
JP 61134379	A2	19860621	JP 1985-271719	19851204
HU 39436	A2	19860929	HU 1985-4642	19851204
HU 194195	B	19880128		
ES 549579	A1	19870501	ES 1985-549579	19851204
SU 1529317	A3	19891207	SU 1985-3988501	19851204
IL 77230	A1	19900610	IL 1985-77230	19851204
AU 8550816	A1	19870611	AU 1985-50816	19851205
AU 611627	B2	19910620		
ZA 8509329	A	19870826	ZA 1985-9329	19851205
PRIORITY APPLN. INFO.:			US 1984-676745	19841205
			IL 1984-72028	19840605
			EP 1985-115243	19851130

GI



AB Title compds. I (R1 = halo, alkynyl, acyl, etc.; R2 = H, F, Cl, Br, NO2; R1R2 = alkylendioxy; R3 = NH2, acylamino, alkanesulfinylamino, alkanesulfonylamino, etc.), which showed antibacterial activity, were prepd. Thus, 4-ClC6H4NCO was cyclocondensed with epibromohydrin to yield I (R1 = 4-Cl, R2 = H, R3 = Br) which was treated with NaN3, hydrogenated, and acylated with ClCO2Me to give I (R1 = 4-Cl, R2 = H, R3 = NHCO2Me) (II). In mice, II had an ED50 of 79.2 mg/kg orally against Staphylococcus aureus.

IT **96800-17-8P**

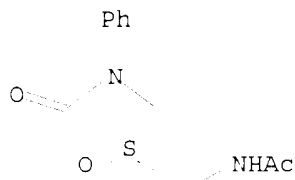
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. and reaction of)

RN 96800-17-8 CAPLUS

CN Acetamide, N-[[[(5S)-2-oxo-3-phenyl-5-oxazolidinyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Golam Shameem



L8 ANSWER 18 OF 19 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1985:437470 CAPLUS

DOCUMENT NUMBER: 103:37470

TITLE: Aminomethyloxooxazolidinylbenzene derivatives useful as antibacterial agents

INVENTOR(S): Gregory, Walter Adelman

PATENT ASSIGNEE(S): du Pont de Nemours, E. I., and Co., USA

SOURCE: Eur. Pat. Appl., 85 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 3

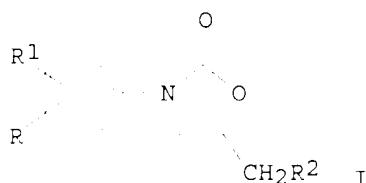
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 127902	A2	19841212	EP 1984-106400	19840605
EP 127902	A3	19870902		
EP 127902	B1	19911016		
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
ES 533097	A1	19850801	ES 1984-533097	19840604
AU 8429099	A1	19841213	AU 1984-29099	19840605
AU 583250	B2	19890427		
IL 72028	A1	19880531	IL 1984-72028	19840605
CA 1254213	A1	19890516	CA 1984-455844	19840605
AT 68490	E	19911115	AT 1984-106400	19840605
FI 8402273	A	19841208	FI 1984-2273	19840606
FI 83216	B	19910228		
FI 83216	C	19910610		
DK 8402795	A	19841208	DK 1984-2795	19840606
NO 8402273	A	19841210	NO 1984-2273	19840606
NO 163451	B	19900219		
NO 163451	C	19900530		
JP 60008277	A2	19850117	JP 1984-114710	19840606
HU 34462	A2	19850328	HU 1984-2192	19840606
HU 194194	B	19880128		
ZA 8404265	A	19860129	ZA 1984-4265	19840606
HU 196771	B	19890130	HU 1987-5132	19840606
SU 1505442	A3	19890830	SU 1984-3752502	19840606
ES 540812	A1	19880316	ES 1985-540812	19850228
SU 1426451	A3	19880923	SU 1986-4024095	19860207
CA 1275652	A2	19901030	CA 1988-580778	19881020
NO 8902178	A	19841210	NO 1989-2178	19890530
NO 169122	B	19920203		
NO 169122	C	19920513		
PRIORITY APPLN. INFO.:			US 1983-501897	19830607
			US 1984-578332	19840214
			CA 1984-455844	19840605
			EP 1984-106400	19840605

NO 1984-2273  
CA 1985-455844

19840606  
19850402

GI



AB The bactericidal oxazolidinones I [R = e.g. NO<sub>2</sub>, cyano, HO, HS, (un)substituted amines, alkylsulfonyl, alkylthio, alkylsulfinyl, aryl, sulfamoyl, alkoxy, or carbamoyl; R<sub>1</sub> = H, F, Cl, Br, NO<sub>2</sub>; RR<sub>1</sub> = alkylenedioxy, R<sub>2</sub> = NH<sub>2</sub>, acylamino, N<sub>3</sub>, alkylsulfonylamino, alkylsulfinylamino] and their physiol. acceptable salts were prepd. Thus, (.-.-)-I (R = 4-MeSO<sub>2</sub>, R<sub>1</sub> = H, R<sub>2</sub> = Cl) was treated with NaI and the resulting (.-.-)-I (R<sub>2</sub> = iodo) treated with NaN<sub>3</sub> followed by hydrogenation in F<sub>3</sub>CCO<sub>2</sub>H to give (.-.-)-I (R-4-MeSO<sub>2</sub>; R<sub>1</sub> = H, R<sub>2</sub> = NH<sub>2</sub>).F<sub>3</sub>CCO<sub>2</sub>H (II). The min inhibitory concn of II was 50 µg/mL against *Staphylococcus epidermidis*.

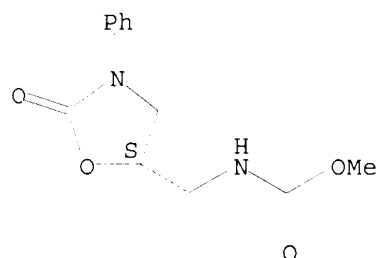
IT **96800-18-9P 96800-36-1P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)  
(prepn. and chlorosulfonylation of)

RN 96800-18-9 CAPLUS

CN Carbamic acid, [(2-oxo-3-phenyl-5-oxazolidinyl)methyl]-, methyl ester,  
(S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

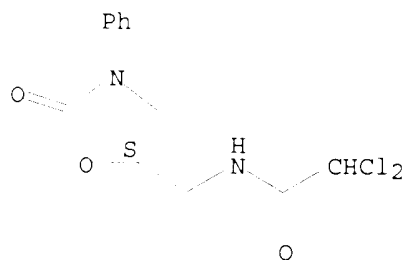


RN 96800-36-1 CAPLUS

CN Acetamide, 2,2-dichloro-N-[(2-oxo-3-phenyl-5-oxazolidinyl)methyl]-, (S)-  
(9CI) (CA INDEX NAME)

Absolute stereochemistry.





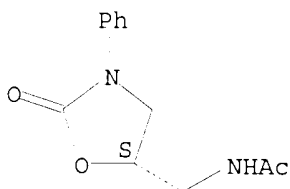
IT 96800-17-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)  
(prepn., nitration, and bactericidal activity of)

RN 96800-17-8 CAPLUS

CN Acetamide, N-[[[(5S)-2-oxo-3-phenyl-5-oxazolidinyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L8 ANSWER 19 OF 19 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1975:72918 CAPLUS

DOCUMENT NUMBER: 82:72918

TITLE: 1,3,5-Substituted dialuric acids

AUTHOR(S): Aspelund, Helge; Waselius, Peter

CORPORATE SOURCE: Org. Chem. Inst., Abo Akad., Turku, Finland

SOURCE: Acta Acad. Abo., Ser. B (1973), 33(20), 34 pp.

CODEN: AAAMA4

DOCUMENT TYPE: Journal

LANGUAGE: German

GI For diagram(s), see printed CA Issue.

AB Alk. hydrolysis of the dialuric acids I (R = CH<sub>2</sub>Ph, Ph, CHMe<sub>2</sub>, Pr) occurred simultaneously at several points in the ring. Cleavage at the 3,4- and 1,6-positions gave tartronuric acids, and cleavage at the 2,3-position led to unstable carbamic acids, which cyclized to 2,4-dioxooxazolidine-5-carboxanilides (II) or cleaved to tartronic acid methylamide anilides. Acetone and alc. promoted the 2,3-cleavage. The tartronuric acids were cyclized in acid medium to N-methyl-2,4-dioxooxazolidine-5-carboxamides, which were cleaved by alkali to tartronic acid methylamide anilides and tartronuric acids, whereas II gave only tartronic acid methylamide anilides.

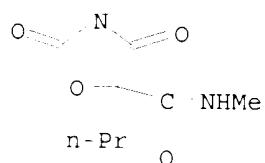
IT 54639-23-5 54787-09-6

RL: PRP (Properties)  
(NMR of)

RN 54639-23-5 CAPLUS

CN 5-Oxazolidinecarboxamide, N-methyl-2,4-dioxo-3-phenyl-5-propyl- (6CI, 9CI)  
(CA INDEX NAME)

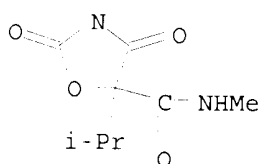
Ph



RN 54787-09-6 CAPLUS

CN 5-Oxazolidinecarboxamide, N-methyl-5-(1-methylethyl)-2,4-dioxo-3-phenyl-  
(9CI) (CA INDEX NAME)

Ph



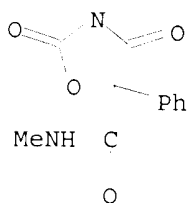
IT 54639-10-0P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

RN 54639-10-0 CAPLUS

CN 5-Oxazolidinecarboxamide, N-methyl-2,4-dioxo-3,5-diphenyl- (6CI, 9CI) (CA  
INDEX NAME)

Ph



=&gt; log y

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

83.79

374.13

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

-11.77

-13.01

STN INTERNATIONAL LOGOFF AT 16:22:11 ON 22 SEP 2002

Golam Shameem